Methyl 4-hydroxy(²H₄)benzoate 362049-51-2 | DTXSID20858080

Model Performance	

Model

Weighted KNN model

Data

5-fold CV (75%)		Training (75%)		Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 266 °C

Global applicability domain: Inside

Local applicability domain index: 7.23e-01

Confidence level: 6.71e-01

Nearest Neighbors from the Training Set

Image not found

Methyl 3-hydroxybenzoate

Measured: 281 Predicted: 266

Image not found

Phenol, 4-chloro-2-methoxy-

Measured: 241 Predicted: 238

Image not found

Ethanone, 1-(3-hydroxyphenyl)-

Measured: 296 Predicted: 270

Image not found

2-Hydroxy-3-

methoxybenzaldehyde

Measured: 266 Predicted: 266